Development of an Integrated Modeling Framework for Simulations of Coastal Processes in Deltaic Environments Using High-Performance Computing

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LONG-TERM GOALS

The long-term goal of our project is to develop and enhance research and educational capabilities in the area of coastal engineering and science at Louisiana State University (LSU) while simultaneously supporting the Navy's research goals in the area of Coastal Geosciences. The focus of the present work is to develop a new modeling framework for simulations of coastal processes in deltaic environments using advanced numerical methods and high performance computing technology. In particular, the utilization of adaptive numerical methods such as the spectral element method on modern computer platforms with thousands of multi-core processors will enable coastal modelers to simulate complex physical processes with improved accuracy and efficiency.

OBJECTIVES

The specific objectives of this project are to:

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- Develop the capability of modeling coastal circulation and nearshore surface waves in deltaic sedimentary and hydrodynamic environments in an integrated modeling framework by extending the Boussinesq theory for nearshore hydrodynamics to muddy coasts and non-hydrostatic three-dimensional (3D) flow regimes with stratifications.
- Apply advanced high-order numerical methods to coastal hydrodynamic modeling.
- Simulate large-scale, long-term problems in the deltaic environment by integrating the application-oriented modeling system with massive-processor computing facilities and technologies available at LSU.
- Complement the Office of Naval Research recent research initiatives on Tidal Flats and Wave-Mud Interactions by integrating the new modeling system with the field data collected in those programs.

APPROACH

The research project consists of theoretical formulation and analysis, the development and verification of an advanced modeling system using the spectral/hp element methods and high-performance computing technologies, and the utilization of the new model as a research tool to advance knowledge and understanding of coastal circulation and nearshore waves in deltaic sedimentary and hydrodynamic environments. Relevant methodologies in three disciplines: civil engineering, physical oceanography and computational science, are being utilized. Interdisciplinary interactions are taking place among the investigators in different fields and through recruiting graduate students from the three disciplines. All project members meet together weekly, with meetings alternating between focusing on coastal science and computational science. Code development and document preparation is enabled through a project-wide source code versioning system.

A new approach is taken to meet the objectives of this project: 1) Use the Boussinesq theory (e.g., Chen 2006) to improve the efficiency of non-hydrostatic 3D Navier-Stokes equation solvers as well as to extend the applicability of the modeling system to deltaic environments, and 2) utilize spectral/hp element methods with unstructured grids to solve the partial differential equations (PDE) under realistic deltaic conditions on high-performance, massive-processor computers available at LSU.

Boussinesq-type models for breaking-driven currents in a large nearshore area are computationally demanding. Taking seabed conditions into account by the Boussinesq model will further increase the computational effort by a factor of two. It is therefore desired to speed up Boussinesq models for practical applications, in particular for morphological and ecological simulations. In addition, a direct solution to the Euler equations of motion for coastal waves and currents is also desirable for fully dispersive waves and currents with strong vertical shears. The solution to the growing demand of computing power by coastal models is the use of high-performance computing (HPC) technologies.

WORK COMPLETED

Wave attenuation and mass transport of a water-mud system due to a solitary wave on the free surface has been modeled by using the Chebyshev-Chebyshev collocation spectral method for spatial discretization and a fourth-order multi-stage scheme for time integration. The governing equations were formulated in Lagrangian coordinates and perturbation equations for shallow water waves were

derived. An iteration-by-subdomain technique was introduced to tackle the interface in the two-layer system. The numerical model was tested against available analytical solutions and good agreement has been found. Although the model is focused on solitary waves and Newtonian fluid-mud, the methodology can be extended to oscillatory, nonlinear water waves over a non-Newtonian mud bottom.

The Boussinesq approach has been applied to a three-dimensional Euler solver for highly dispersive waves and stratified flows. Free from the irrotational flow assumption, the three-layer model can correctly resolve the free-surface displacement and the velocity profile of short waves interacting with shear currents, which cannot be easily obtained by the existing Boussinesq-type equations.

Considerable effort has been devoted to the implementation of the discontinuous Galerkin scheme using the open-source spectral/*hp* library Nektar++ (www.nektar.info) and its predecessor, Nektar. Through Nektar++/Nektar, the fundamental routines associated with a high-order finite-element method are easily accessible. We have solved the nonlinear shallow water equation, the Boussinesq-type equations for waves and currents, and the Euler equations of motion on the vertical plane based on spectral element/hp discontinuous Galerkin methods. Testing of the codes is being conducted.

Our approach in parallelizing the shallow water equation (SWE) solver was to integrate our code into the Cactus computational framework (Goodale et al. 2003) and provide parallelism through a Cactus "Driver" module (or "thorn''). Cactus (www.cactuscode.org) is an open source problem solving environment designed for scientists and engineers. Its modular structure easily enables parallel computation across different architectures and collaborative code development between different groups. Cactus originated in the academic research community, where it was developed and used over many years by a large international collaboration of physicists and computational scientists.

In order to integrate the serial SWE solver into Cactus, several thorns have been developed. Most importantly, we have designed a "Nektar++" thorn that initializes and populates the data structures of Nektar++. We also provide a "SWE" thorn that contains the actual SWE solver based on routines defined in the SWE solver library. Both spectral/ph element SWE and fourth-order finite difference SWE solvers have been integrated with Cactus to take advantage of its parallelism.

RESULTS

The major results obtained in 2009 are: 1) the development of a high-order numerical model for wave attenuation and mass transport of a wave-mud system due to a solitary wave using the Chebyshev-Chebyshev collocation spectral method for spatial discretization and a fourth-order multi-stage scheme for time integration, 2) the improvement of a three-dimensional (3D) Euler solver for fully dispersive water waves by extending the Boussinesq approach to the treatment of the non-hydrostatic pressure on the top layer of the 3D model, 3) the continued implementation and testing of the Boussinesq model (FUNWAVE) for waves and currents on a solid bed into the Cactus Framework using high-order finite-difference schemes to serve as a verification tool, 4) the implementation of spectral/hp element method for incompressible flow with and without a free surface, and 5) the public release of the Shallow Water Solver as part of the Nektar ++ software package for computational fluid dynamics based on the spectral/hp element method (www.nektar.info).

A Spectral Collocation Model for Solitary Wave Attenuation and Mass Transport over Viscous Mud

The numerical model solves the first- and second-order equations derived from the Navier-Stokes equations for viscous fluid motion in Lagrangian coordinates. Shallow water, week displacement, and a horizontal bed have been assumed in the perturbation analysis for a two-layer Newtonian fluid-mud system on the vertical plane. The numerical model based on the high-order numerical methods has been tested against available analytical solutions and good agreement has been found. Due to the high viscosity of the bottom fluid-mud, the modeled horizontal particle velocities and particle displacements decrease with the distance as the wave propagates, which justifies the use of non-periodic spectral schemes. The computed wave attenuation rate is in good agreement with the analytical solution of Jiang and Zhao (1989) when the thickness of the mud layer is relatively thick. Numerical simulations however suggest that the accuracy of the existing boundary layer theory for wave-mud interaction is limited when the mud-layer thickness becomes smaller than the wave height because the assumed irrotational core may not exist. Although the model has been focused on solitary waves and Newtonian fluid-mud, the modeling framework developed can be extended to oscillatory, nonlinear waves over a non-Newtonian mud bottom modeled as a power-law fluid. The result was published in the Journal of Engineering Mechanics (Huang and Chen 2009).

Improvement of an Euler Solver for Fully Dispersive Water Waves Using the Boussinesq Approach

The basic idea to improve the accuracy of a three-dimensional Euler solver for fully dispersive waves is to obtain an analytical-based form of non-hydrostatic pressure distribution at the top layer by using the principle of Boussinesq theory: 1) The vertical profiles of horizontal velocity components are obtained by using the Taylor series expansion at the reference location; 2) the vertical velocity profile is obtained by substituting the horizontal velocity components into the continuity equation and integrating the resulting equation from the reference to an arbitrary location z ; and 3) the analytical form of pressure profile is obtained by integrating the vertical momentum equation from an arbitrary z to the free surface and applying the Leibniz's rule with the use of free-surface kinematic boundary condition and free-surface pressure condition. Numerical experiments have shown that this Boussinesq-like treatment of the top layer enables the use of as few as four vertical layers to accurately model nonlinear short waves with dimensionless wave number, kh=16, which can not be easily simulated by existing Boussinesq-type models. Different from conventional Boussinesq models, the integration in the vertical direction is only limited to the top layer and no assumption of zero horizontal vorticity components was made. The result will appear in the Journal of Waterway, Port, Coastal and Ocean Engineering (Wu et al. 2010).

A Highly Parallelized Shallow Water Wave Solver Based on Combined OpenMP and MPI

As part of the continued development of the parallel Boussinesq model for waves and currents within the Cactus Framework using high-order finite-difference schemes, a combined OpenMP and MPI have been used to speed up the code. We used 4th order central differencing for spatial discretization and 4th order Runge-Kutta method for time integration. A ShallowWater thorn (or module) implemented in Cactus uses Carpet as the parallel driver. Figure 1 shows the result of weak scaling test of the shallow water wave solver for wave sloshing in a rectangular tank. The number of processors ranges from 4 cores (1 node) to 256 cores. The mesh size was 1004x1004 (including the grid points used for imposing the wall boundary conditions) in the x- and y-direction for the 4 core job and increased proportionally as the number of cores increases. The computational work per core is maintained constant and the total size of the problem increases with increase in number of processors (weak

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scaling). For an ideal weak scaling, the time to the solution should not increase significantly when the problem size is increased in proportion to the number of processors. All these tests were performed on the "Painter" supercomputer (www.loni.org) that has 680 nodes with each node having 2 quad-core processor (i.e. 8 cores) with 8 Gb RAM. It is seen in Figure1 that good scaling has been achieved up to 256 cores which was the limit of these initial experiments. Since the Cactus parallel drivers have already been shown to scale to over 130,000 cores with single grid finite difference problems we expect this scaling to continue. The variance in the scaling seen in the graph is likely due to the changing topology of the decomposition of the computational grid across the cores which causes variations in the local grid sizes on each core. The different lines on the graph relate to the different numbers of OpenMP threads used.
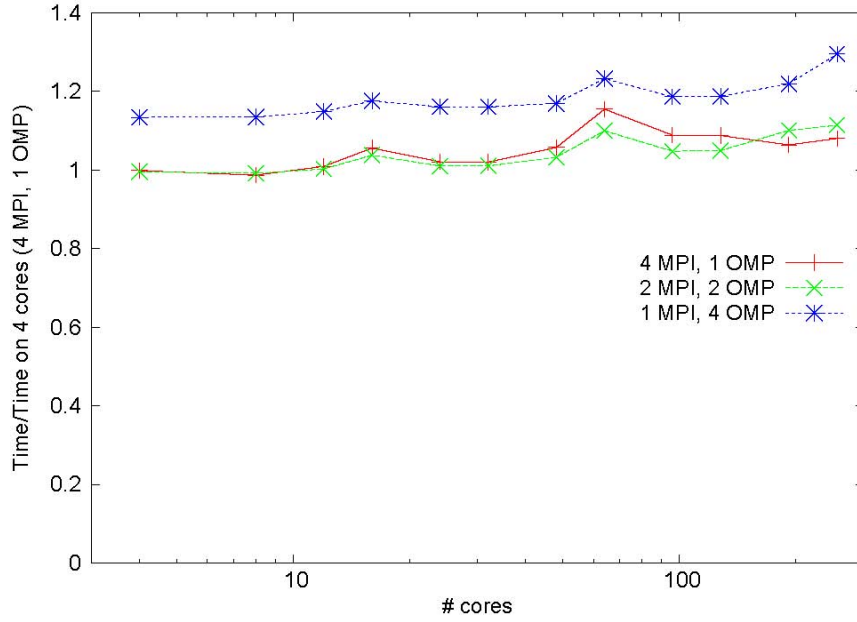

Figure 1 *Weak scaling tests of the shallow water wave solver in Cactus.*

Continuous and Discontinuous Galerkin Spectral/hp Element Methods for Incompressible Flows

For complex 3D flow problems with strong vertical variations, a direct solution to Euler equation or Navier-Stokes (N-S) equation is desirable. Basically, there are two approaches for solving the pressure field applied to incompressible flow problems in an Euler solver. The first method is to solve the Helmholtz or Possion equation to obtain the pressure field (e.g., Karniadakis and Sherwin 2005) and the second one is the artificial compressibility (AC) method first proposed by Chorin (1967). The attributes of AC methods are its high efficiency (less memory requirement compared to directly solving Helmholtz equation), parallel computing, and its robustness for complicated flow problems. The implementation of AC method is relative simple. Comparisons of both approaches in the context of discontinuous Galerkin spectral/hp element methods for water waves are being carried out.

In order to simulate nonlinear water waves, the arbitrary Lagrangian-Eulerian (ALE) method is utilized to handle the moving free surface in the current spectral element code. ALE is a well-documented algorithm for moving domain and deformation problems (Hirt et al. 1974). We are benchmarking the

code to determine the performance of the ALE for highly nonlinear water wave problems solved by spectral/hp element methods.

The spectral/hp element solver for the N-S equation is being tested and the preliminary results are shown in Figures 2-6. The first test case is a backward-facing flow (channel flow) in which the step is a half height of the channel width (Figure 2). As observed in many experiments, the steady discharge in the upstream produces a large re-circulation zone attached to the backward-facing step, which is a useful test case for numerical models. Figures 3-4 illustrate the computed flow separation and the resultant velocity and pressure fields.
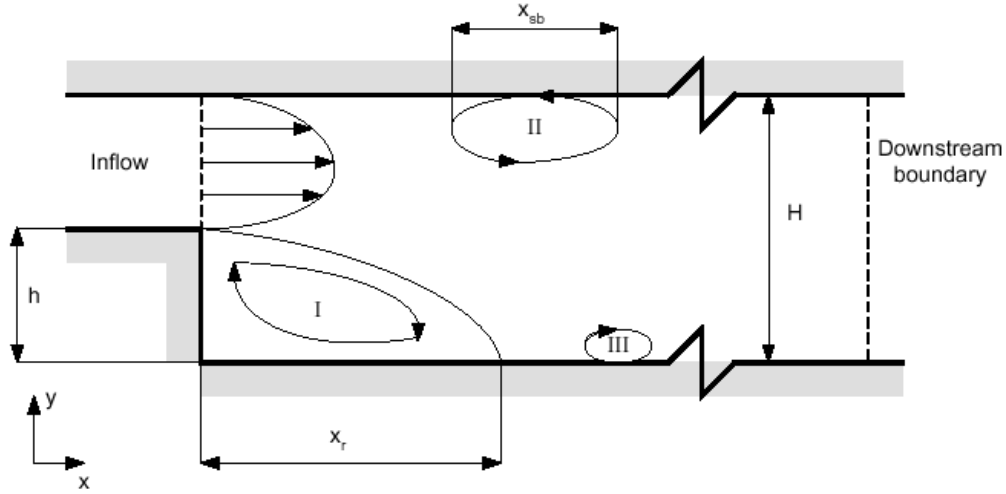

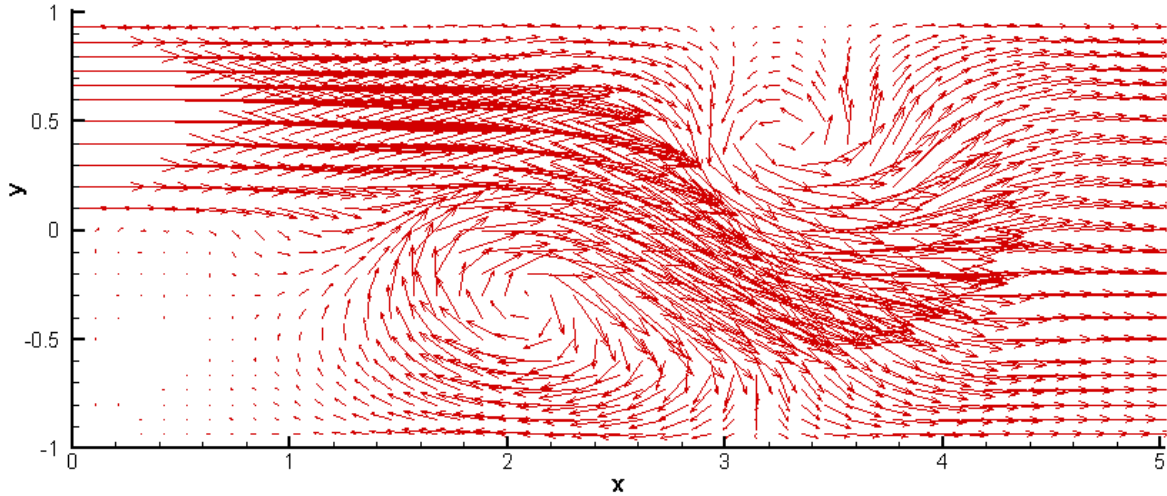**Figure 2** *Schematic of a backward facing flow setup for benchmarking the spectral/hp element model.*

Figure 3 *Modeled velocity vectors of the backward-facing flow at Re=1000 using quadrilateral elements at a transition state (t=4 s). The inlet velocity is u= 2.0 m/s and v=0.0 m/s, and the downstream boundary is non-reflective.*
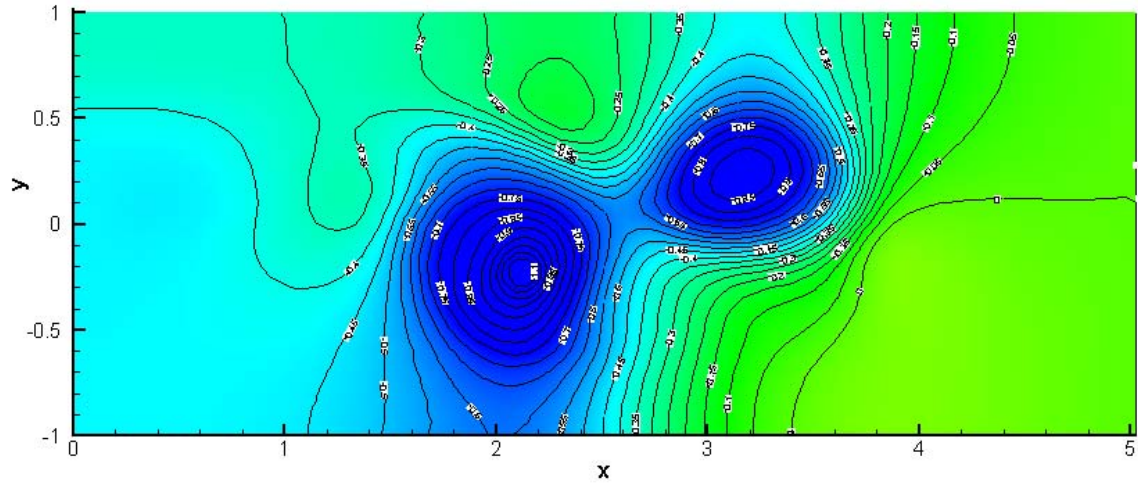
Figure 4 *Pressure contours for a backward facing flow at Re=1000 and t=4s as in Figure 3.*

The second test case is an incompressible flow passing a horizontal circular cylinder. Unstructured triangular elements are applied in the computational domain with curved edges/surfaces. Numerical results from the spectral/hp element code show that the vertex shedding starts at Re=116, which is in very good agreement with other finite element simulations with much finer spatial resolution (e.g., Kundu and Cohen 2002). More quantitative comparisons between the results from the new solvers and available analytic solution and experimental data are underway.
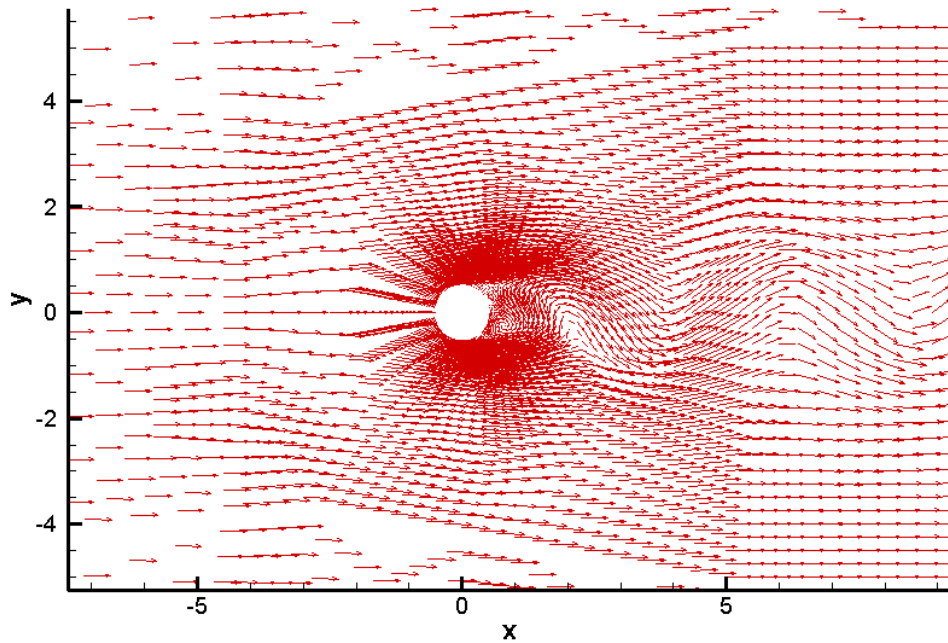

Figure 5 *Computed Vortex shedding by the spectral/hp element method with unstructured triangular elements at Re=150. The shedding starts at Re=116, which is very close to the result of a body-fitted finite element simulation with finer resolution (Kundu and Cohen, 2002).*
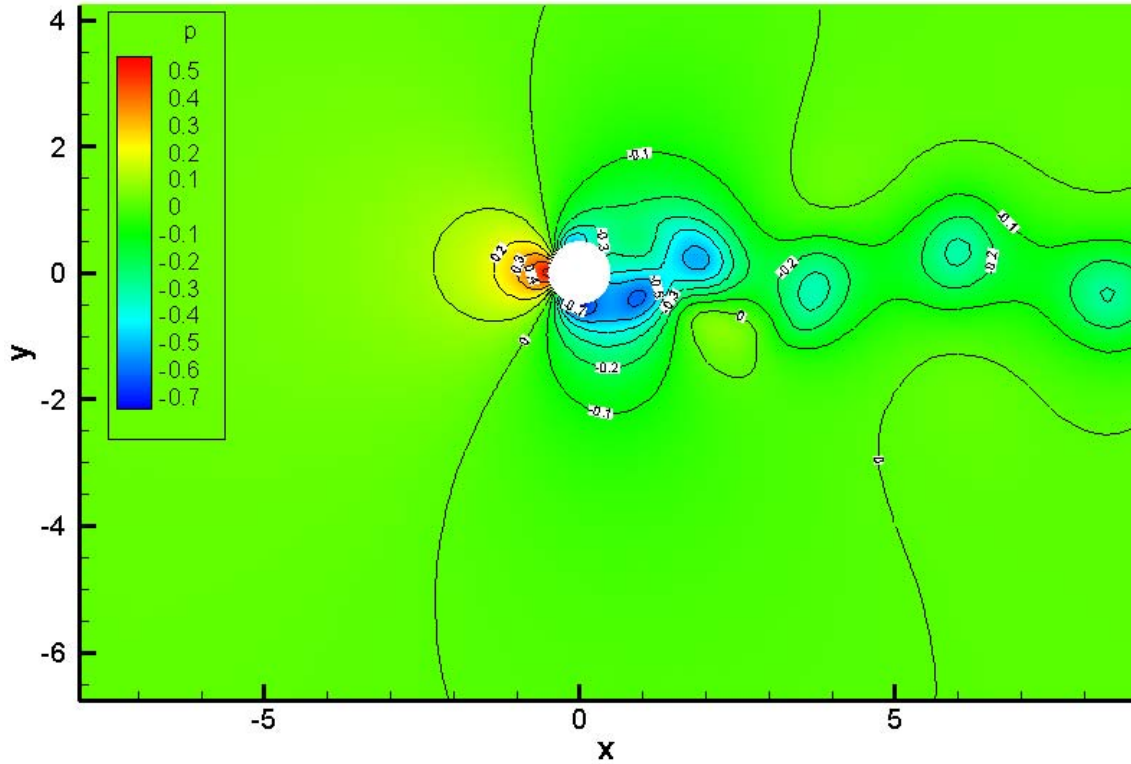
Figure 6 *Computed pressure contours of the flow passing a horizontal cylinder at Re=150.*

Public Release of the Discontinuous Galerkin Shallow Water Solver in Nektar ++

The close collaboration between the LSU's team and the Nektar ++ developers (Prof. Spenser Sherwin and his team) at the Imperial College London, U.K. has resulted in the public release of the Spectral/hp element discontinuous Galerkin (DG) shallow water solver (SWS) developed though this project as part of the latest version of the Naktar ++ software package for computational fluid dynamics (www.nektar.info). The DG SWS class contains functions for the evaluation of the flux vectors, numerical fluxes, equation dependent boundary conditions, various source terms, etc. This class provides a shallow water equation solver library in Nektar++. Details on the numerical implementation of the DG SWS have been documented in Eskilsson et al. (2009).

IMPACT/APPLICATIONS

We have successfully implemented a spectral/*hp* discontinuous Galerkin method for solving the SWE and interfaced it with the Cactus computational framework. The DG shallow water solver has become a part of the Nektar++ package for CFD available to the public. We have also developed a spectral model to study wave and mud interaction, and have improved the accuracy of a 3D Euler solver for highly dispersive waves. We have obtained encouraging results in terms of parallel performance and the coupled software's scaling ability. The use of Cactus provides a path for extensibility, integrating with cutting-edge computational hardware and cyberinfrastructure, and building a comprehensive toolkit for coastal applications. The results were documented in the recent publications (Huang and Chen 2009, Wu et al. 2010, and Eskilsson et al. 2009).

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The research is expected to improve the Navy's capability of modeling nearshore surface waves and coastal processes in heterogeneous sedimentary environments. The modeling framework integrated with the CFD Toolkits developed at LSU will allow us to improve the accuracy of hydrodynamic models and couple them with sediment transport models for coastal morphodynamic studies.

In addition to supporting the Navy's research goals, the proposed project is contributing to the Louisiana State University's mission on research and graduate education. The north Gulf Coast, where the Naval Research Laboratory and other naval facilities are located, is in need of research and education in coastal engineering. The training of post-doctoral fellows and graduate students will enhance the graduate grogram in coastal engineering at LSU to meet the need for graduate education on the Gulf Coast in support of national defense.

TRANSITIONS

The spectral/hp element discontinuous Galerkin shallow water solver developed through this project became a part of the open source Nektar++ software package for computational fluid dynamics available to the public (www.nektar.info).

RELATED PROJECTS

Our project is leveraging and coordinating with activities in several other ongoing activities:

XiRel: This NSF funded project is optimizing and extending an Adaptive Mesh Refinement layer for the Cactus framework, which will be used for our structured grid codes. (http://www.cactuscode.org/Development/xirel)

ALPACA: This NSF funded project is developing debugging and profiling tools for the Cactus framework which will support the Coastal Modeling Framework developed in this project. (http://www.cactuscode.org/Development/alpaca)

CyberTools: This NSF/BOR funded project is developing a cyberinfrastructure across the 100 TFlop machines of the Louisiana Optical Network Initiative. Our project is providing one of the application drivers for this infrastructure. (http://cybertools.loni.org)

Blue Waters: This large NSF funded project will deploy a petascale computing facility at NCSA in 2011. Our Cactus-based coastal application will provide a driver problem for the development of software for this resource.

CFD IGERT: An NSF graduate training and education program at LSU in training students in computational fluid dynamics and high performance computing. Several research projects are building on the CFD Toolkit which is contributing to our project.

SCOOP: Where appropriate, our models will be integrated into the community infrastructure of the NOAA/ONR funded SURA Coastal Ocean and Observing Program. SCOOP maintains a coastal archive at LSU with realtime forcing and simulation data for storm events.

NSF-CAREER: The five-year research project is focused on simulations of nonlinear coastal waves and air-sea momentum fluxes, which complements the present research project. (http://www.nsf.gov/eng/cbet/nuggets/1443/1443_chen.htm)

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